

Benzoic acid, 2,3-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester

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|-----------------------------|--|
| Other names: | Benzoic acid, 2,3-dihydroxy, tri-TMS Benzoic acid, 2,3-dihydroxy, TMS 2,3-Dihydroxybenzoic acid, 3tms derivative |
| Inchi: | InChI=1S/C16H30O4Si3/c1-21(2,3)18-14-12-10-11-13(15(14)19-22(4,5)6)16(17)20-23(7) |
| InchiKey: | IPIPJXIWUUYKNS-UHFFFAOYSA-N |
| Formula: | C16H30O4Si3 |
| SMILES: | C[Si](C)(C)OC(=O)c1cccc(O[Si](C)(C)C)c1O[Si](C)(C)C |
| Mol. weight [g/mol]: | 370.66 |
| CAS: | 3618-19-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 1.38 | | Crippen Method |
| logp | 5.106 | | Crippen Method |
| rinpol | 1743.00 | | NIST Webbook |
| rinpol | 1744.00 | | NIST Webbook |
| rinpol | 1728.40 | | NIST Webbook |
| rinpol | 1749.00 | | NIST Webbook |
| rinpol | 1749.00 | | NIST Webbook |
| rinpol | 1728.40 | | NIST Webbook |
| rinpol | 1743.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3618197&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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